

# AUTOMATED POSITIVE PART EXTRACTION FOR LATTICE PATH GENERATING FUNCTIONS IN THE OCTANT

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ABSTRACT. The question of classifying the nature of the generating functions of restricted lattice walks has enjoyed much attention in past years. We prove that a certain class of octant walks have a D-finite generating function using the theory of multivariate formal Laurent series.

## 1. INTRODUCTION

We focus our attention in this paper to the *positive octant*, i.e., the three-dimensional integer lattice, restricted so that all coordinates are nonnegative.

Let  $\mathcal{L} = (\mathbb{Z}_{\geq 0})^3$ . Fix a *model* (also called *stepset*)  $\mathcal{S} \subset \{-1, 0, 1\}^3 \setminus \{(0, 0, 0)\}$ . A length  $m$   $\mathcal{S}$ -walk is any walk which starts at  $(0, 0, 0)$  and takes  $m$  steps from  $\mathcal{S}$ . Let  $f(i, j, k; n)$  denote the number of  $\mathcal{S}$ -walks of length  $n$  ending at point  $(i, j, k) \in \mathcal{L}$ . We form the generating function

$$F(x, y, z; t) = \sum_{i, j, k, n \geq 0} f(i, j, k; n) x^i y^j z^k t^n$$

and ask whether  $F(x, y, z; t)$  is D-finite over  $\mathbb{Q}(x, y, z, t)$  in each variable. In other words, does there exist a nontrivial linear differential equation in each variable with coefficients in  $\mathbb{Q}[x, y, z, t]$ ?

There are  $2^3 - 1 = 67,108,864$  models in the octant. After choosing a canonical representative for models that are in bijection to each other for simple reasons and removing all cases that are equivalent to lower-dimensional problems, we are still left with 10,908,263 models [2]. In [3, 2], these remaining models were sorted according to properties that sometimes help establish whether the corresponding generating function is D-finite. One of these properties is the order of a certain group of rational transformations associated to the model. If the *group of the model* is finite, then it may be possible to establish the D-finite nature of the generating function via the orbit sum argument of [6] (summarized in the next section). There are altogether 2,430 models with a finite group [2, 8]. For 108 of them, it was shown in [3] that their corresponding generating functions are D-finite. We show in the present paper that the orbit sum argument applies to 1,964 additional models, and that they are therefore also D-finite. The remaining 358 models are the *zero orbit sum cases*, for which different methods are needed.

## 2. THE ORBIT SUM METHOD

For a fixed model  $\mathcal{S}$ , we define the *stepset (Laurent) polynomial* to be  $P_{\mathcal{S}} = \sum_{(u, v, w) \in \mathcal{S}} x^u y^v z^w$ . The rational transformation  $\phi_x : \mathbb{Q}(x, y, z) \rightarrow \mathbb{Q}(x, y, z)$  given

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by  $\phi_x(x, y, z) := \left( x^{-1} \frac{\sum_{(-1, v, w) \in \mathcal{S}} y^v z^w}{\sum_{(1, v, w) \in \mathcal{S}} y^v z^w}, y, z \right)$  fixes  $P_{\mathcal{S}}$  as well as  $y$  and  $z$ , and is idempotent. The transformations  $\phi_y$  and  $\phi_z$  are defined similarly. Then, the group  $G_{\mathcal{S}}$  generated by  $\phi_x, \phi_y, \phi_z$  via composition is called the *group of the model* [6, 3]. For  $g \in G_{\mathcal{S}}$ ,  $\text{sgn}(g) = 1$  if  $g$  is a composition of an even number of generators, and  $-1$  otherwise.

Most models in the octant have an infinite group, but for the 2,430 cases in the octant with a finite group, we can attempt to use the *orbit sum method* to prove that their corresponding generating functions are D-finite. The details of this technique for the octant appear in [3]; we reproduce a brief sketch here.

The starting point of the technique is the *functional equation*, which can be obtained using an inclusion-exclusion argument. The left-hand side of this equation only involves  $F(x, y, z; t)$ , but the right-hand side involves *sections* or *specializations* of  $F(x, y, z; t)$  such as  $F(x, y, 0; t)$  and  $F(x, 0, 0; t)$  [3, Eqn. 7]. Using the group of the model, we form the *orbit sum*, which allows us to eliminate the sections on the right-hand side and leaves us with:

$$\sum_{g \in G} \text{sgn}(g) g(xyz) (F(g(x), g(y), g(z); t)) = \frac{1}{1 - tP_{\mathcal{S}}} \sum_{g \in G} \text{sgn}(g) g(xyz) \quad (1)$$

The generating function  $F(x, y, z; t)$  is an element of  $\mathbb{Q}[x, y, z][[t]]$ . Thus,  $F_g := F(g(x), g(y), g(z); t) \in \mathbb{Q}(x, y, z)[[t]]$  is a power series in  $t$  with coefficients  $a_i \in \mathbb{Q}(x, y, z)$ . We regard each of these  $a_i$  as a *multivariate formal Laurent series* rather than a rational function (see Section 3). Then, the positive part extraction  $[x^{>0} y^{>0} z^{>0}]$  is well-defined, and we apply it to obtain an expression with only  $F(x, y, z; t)$  on the right-hand side

$$xyz F(x, y, z; t) = [x^{>0} y^{>0} z^{>0}] \frac{1}{1 - tP_{\mathcal{S}}(x, y, z)} \sum_{g \in G} \text{sgn}(g) g(xyz) \quad (2)$$

The above equation holds if every monomial in  $F_g$  has at least one negative component in its exponent for each non-identity element  $g \in G_{\mathcal{S}}$ . Then,  $F(x, y, z; t)$  can be written as the diagonal of a rational series, and is therefore D-finite [4, 10].

The orbit sum technique gives a uniform method for proving that some octant models have D-finite generating functions. However, it is not without its limitations. If there are one or more non-identity  $g \in G_{\mathcal{S}}$  such that  $F(g(x), g(y), g(z); t)$  contributes to the positive part on the left-hand side, we do not obtain an expression for  $xyz F(x, y, z; t)$  alone, and therefore cannot conclude that  $F(x, y, z; t)$  is D-finite. For such models, a different proof technique is needed. Included among these models are the so-called *zero orbit sum* cases, for which the right-hand side of Equation 1 is 0. In the quadrant, these models correspond exactly to the cases where the generating function is algebraic [6, 5]. In the octant, there are two subclasses among the zero orbit sum cases: *Hadamard* and “mysterious”. Bostan et al provide an alternative proof technique for octant Hadamard cases in [3]: all of the zero orbit sum Hadamard models they consider have D-finite generating functions. The remaining 170 models are those which were deemed “mysterious” in [2]. These cases have yet to be definitively classified, but there is strong computational evidence that at least some of them have non-D-finite generating functions [2].

In this paper, we identify models for which  $xyz F(x, y, z; t)$  is the only surviving term on the left-hand side of Equation 1 after the positive part extraction, and

prove automatically that their generating functions are D-finite via the orbit sum argument.

### 3. MULTIVARIATE FORMAL LAURENT SERIES

We recall here the bare essentials of the theory of multivariate formal Laurent series, as formalized by Aparicio-Monforte and Kauers [1]. In order to ensure that multiplication of series is well-defined, we consider multivariate series with support contained in a *line-free* cone.

Let  $k$  be a field,  $x_1, \dots, x_n$  be  $n$  indeterminates, and  $C \subset \mathbb{R}^n$  be a line-free cone.  $k_C[[x_1, \dots, x_n]] := \{f(\mathbf{x}) = \sum_{\mathbf{k}} a_{\mathbf{k}} \mathbf{x}^{\mathbf{k}} \mid \text{supp } f(\mathbf{x}) \subseteq C\}$  with the usual addition and Cauchy product multiplication is an integral domain. If, on the other hand, we fix a specific additive order on  $\mathbb{Z}^n$ , we can form the sets  $k_{\preceq}[[\mathbf{x}]] := \bigcup_{C \in \mathcal{C}} k_C[[\mathbf{x}]]$  and  $k_{\preceq}((\mathbf{x})) := \bigcup_{\mathbf{v} \in \mathbb{Z}^p} \mathbf{x}^{\mathbf{v}} k_{\preceq}[[\mathbf{x}]]$ , where  $\mathbf{x} = (x_1, \dots, x_p)$  with  $x_i$  indeterminate for every  $i$ , and  $\mathcal{C}$  is the set of all cones  $C \subset \mathbb{R}^p$  compatible with  $\preceq$ . The condition that  $\preceq$  be additive ensures that  $k_{\preceq}[[\mathbf{x}]]$  is a ring and that  $k_{\preceq}((\mathbf{x}))$  is a field [1, Thm. 15]. We call  $k_{\preceq}[[\mathbf{x}]]$  a multivariate formal Laurent series ring and  $k_{\preceq}((\mathbf{x}))$  the field of the multivariate formal Laurent series ring. We define the *leading exponent* of an element  $f(\mathbf{x})$  to be  $\text{lexp}_{\preceq} f(\mathbf{x}) = \min_{\preceq}(\text{supp } f(\mathbf{x})) \in \mathbb{Z}^p$ , and the *leading term*  $\text{lt}_{\preceq} f(\mathbf{x}) = \mathbf{x}^{\text{lexp}_{\preceq} f(\mathbf{x})}$ .

The following theorem is essential for the automatic positive part extraction we will describe in the next section:

**Theorem 1** ([1, Thm. 17]). *Let  $C \subset \mathbb{R}^q$  be a line-free cone and  $f(\mathbf{y}) \in k_C[[y]]$ . Let  $\preceq$  be an additive order on  $\mathbb{Z}^p$  and  $a_1(\mathbf{x}), \dots, a_p(\mathbf{x}) \in k_{\preceq}((\mathbf{x})) \setminus \{0\}$ . Let  $M \in \mathbb{Z}^{p \times q}$  be the matrix whose  $i^{\text{th}}$  column consists of the leading exponent  $\text{lexp}(a_i(\mathbf{x}))$ . Let  $C' \subset \mathbb{R}^p$  be a cone containing  $MC := \{M\mathbf{x} \mid \mathbf{x} \in C\} \subset \mathbb{R}^p$  as well as  $\text{supp}(a_i(\mathbf{x})/\text{lt}(a_i(\mathbf{x})))$  for every  $i \in \{1, \dots, q\}$ . Suppose that  $C \cap \ker M = \{\mathbf{0}\}$  and that  $C'$  is line-free. Then,  $f(a_1(\mathbf{x}), \dots, a_p(\mathbf{x}))$  is well-defined and belongs to the ring  $k_{C'}[[\mathbf{x}]]$ .*

After the positive part extraction is applied with the help of this theorem, the next step is to find a differential equation for  $F(x, y, z; t)$  and possibly an expression for  $F(x, y, z; t)$  itself. The theory of multivariate formal Laurent series is also useful for this step: in [4], for example, this theory is used to prove computationally guessed annihilating differential operators for the sections  $F(x, 0; t)$  and  $F(0, y; t)$  of certain quadrant models. These operators lead to an annihilating differential operator for  $F(x, y; t)$ , as well as explicit expressions for  $F(x, y; t)$  in terms of hypergeometric functions.

### 4. APPLICATION TO LATTICE PATHS

For a given  $\mathcal{S}$ , we apply Theorem 1  $|G_{\mathcal{S}}|$  times. The support of  $F(x, y, z; t)$  can be shown to be contained in  $C = \langle (1, 0, 0, 1), (0, 1, 0, 1), (0, 0, 1, 1), (0, 0, 0, 1), (1, 1, 0, 1), (1, 0, 1, 1), (0, 1, 1, 1), (1, 1, 1, 1) \rangle$ . Fix a non-identity  $g \in G_{\mathcal{S}}$ . We set  $f(\mathbf{y}) = F(x, y, z; t)$ ,  $a_1(\mathbf{x}) := g(x)$ ,  $a_2(\mathbf{x}) := g(y)$ ,  $a_3(\mathbf{x}) = g(z)$ , and  $a_4(\mathbf{x}) = t$ . To create an additive order on  $\mathbb{Z}^p$ , we collect all polynomials  $q_i$  that appear in the numerator or denominator of the  $a_i$ . For each of these polynomials  $q_i$  we choose a leading term, and check that this choice of leading term is compatible with the cone. If so, we check the conditions of Theorem 1 are fulfilled. If they are, we conclude that the composition  $F_g = F(g(x), g(y), g(z); t)$  is valid, and also obtain a cone  $C'_g$  with the property that  $F_g \in k_{C'_g}[[\mathbf{x}]]$ . Next, define  $B$  to be the smallest cone

containing  $C$  and  $C'_g$ . We check that  $B$  is line-free, and that  $\text{supp}(g(xyz)F_g) \cap C = \emptyset$ . Then, we have proven that  $[x^{>0}y^{>0}z^{>0}]g(xyz)F_g = 0$ .

If we experience a failure at any of the above steps, we simply choose different leading terms for the  $q_i$  and try again. The properties of  $G_S$  ensure that there are not many polynomials  $q_i$  for which we can choose leading terms, and that each  $q_i$  can only contain a small number of monomials. Thus, it is computationally feasible to check every combination of leading terms that is compatible with  $C$ .

We repeat this process for every non-identity  $g \in G$ , setting  $B$  to be equal to the smallest cone containing the previous cone  $B$  and the cone  $C'_g$ . If the process terminates successfully, we obtain a cone  $B$  with the property that  $g(xyz)F_g \in k_{\leq}(\langle \mathbf{x} \rangle)$  for every  $g$ . We also know that the only contribution to the left-hand side of the orbit sum with support intersecting  $C$  is the element  $xyzF(x, y, z)$ . That is, the positive part extraction step yields an expression for  $xyzF(x, y, z; t)$  alone that allows us to conclude that  $F(x, y, z; t)$  is D-finite.

**Example 1.** Let  $\mathcal{S} = \{(-1, -1, 0), (-1, 0, 1), (-1, 1, -1), (0, -1, 1), (0, 0, -1), (0, 1, 0), (1, 0, 0)\}$ .  $G_S = \langle \phi_x, \phi_y, \phi_z \rangle \cong D_{12}$ , with  $\phi_x = \left(\frac{yz^2+y^2+z}{xyz}, y, z\right)$ ,  $\phi_y = \left(x, \frac{z}{y}, z\right)$ ,  $\phi_z = \left(x, y, \frac{y}{z}\right)$ . For this example, the only polynomial that appears as a term in a rational transformation is  $p = yz^2 + y^2 + z$ . Choose  $\text{lex}_{\leq}(p) = (0, 1, 2, 0)$ . For each  $g \in G$  we now attempt to apply Theorem 1. Consider for example the

$$\text{element } \phi_x \in G_S. \quad M = \begin{pmatrix} -1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 1 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}.$$

We have that  $C \cap \ker(M) = \{\mathbf{0}\}$ . Additionally,  $C'_{\phi_x} = \langle (0, -2, 1, 0), (0, -1, 2, 0), (0, 0, 0, 1) \rangle$ . Thus,  $F_{\phi_x} = \frac{yz^2+y^2+z}{xyz}yzF\left(\frac{yz^2+y^2+z}{xyz}, y, z; t\right)$  is well-defined, and additionally  $\text{supp}(\phi_x(xyz)F_{\phi_x}) \cap C = \emptyset$ . Moreover, the smallest cone  $B$  containing both  $C$  and  $C'_{\phi_x}$  is line-free. Continuing this process for each  $g \in G_S$ , we obtain the cone  $C_G = \langle (1, 1, 1, 1), (1, -1, 2, 1), (0, 1, -2, 0), (-1, -1, 3, 1), (0, -1, -1, 0), (-1, 1, 2, 1) \rangle$ , which is line-free. The left-hand side of the orbit sum equation is well-defined in  $k_{C_G}[[\mathbf{x}]]$ , and  $F(x, y, z; t)$  is the only term that survives the operation  $\text{supp}(g(xyz) \cdot F(g(x), g(y), g(z); t)) \cap C$  for  $g \in G_S$ , and  $F(x, y, z; t)$  is D-finite.

**Example 2.** Next we consider a case for which the right-hand side of Equation 1 is equal to zero. Let  $\mathcal{S} = \{(-1, -1, -1), (-1, 0, 0), (-1, 0, 1), (-1, 1, 0), (1, -1, 0), (1, 0, -1), (1, 1, 1)\}$ .  $G_S \cong D_{12}$  as before, but is generated by different rational transformations  $\phi_x, \phi_y, \phi_z$  than in the previous example. In particular, we have  $\phi_z\phi_y\phi_z = (x, z, y)$ . Since  $\text{lt}_{\leq}(x) = x$ ,  $\text{lt}_{\leq}(y) = y$  and  $\text{lt}_{\leq}(z) = z$  for any choice of  $\leq$ ,

$$\text{we have } M_{\phi_z\phi_y\phi_z} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \quad \text{Since } C'_{\phi_z\phi_y\phi_z} = C, \text{ the term } xyzF(x, z, y)$$

on the left-hand side of Equation 1 survives the positive part extraction, and we cannot proceed.

## 5. OCTANT CASES WITH FINITE GROUP

Using the technique outlined in the previous section, we obtain the following theorem.

**Theorem 2.** *All 2,072 three-dimensional octant models with finite group and nonzero orbit sum are  $D$ -finite.*

We say that a model is three-dimensional if the condition that  $\sum_{s \in \mathcal{S}} a_s s \geq (0, 0, 0)$  is a truly three-constraint problem. A model defined in the octant need not be three-dimensional; see [3, §2.1, §7.1] for a more extended discussion.

Theorem 2 includes the 108 cases that were already proven in [3]. In [2], it was conjectured that the 1,964 models covered in Theorem 2 could be proved  $D$ -finite by the orbit sum method. The contribution of the current work is to confirm this conjecture. The proof is fully automatic: our implementation of the process outlined in Section 4 uses Sage [7] and requires only the model  $\mathcal{S}$  as input.

The remaining 358 models not covered by Theorem 2 are exactly those for which Equation 1 has a vanishing right-hand side. This shows that the only cases for which the orbit sum technique fails at the positive part extraction step are those that are equivalent to two-dimensional cases with multiplicities, which are discussed in [3, 9].

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